On quantum integrability and Hamiltonians with pure point spectrum

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Abstract

We prove that any n-dimensional Hamiltonian operator with pure point spectrum is completely integrable via self-adjoint first integrals. Furthermore, we establish that given any closed set $\Sigma \subset \mathbb{R}$ there exists an integrable n-dimensional Hamiltonian which realizes it as its spectrum. We develop several applications of these results and discuss their implications in the general framework of quantum integrability.

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1 Introduction

A classical Hamiltonian h, that is, a function from a 2n-dimensional phase space into the real numbers, completely determines the dynamics of a classical system. Its complexity, i.e., the regular or chaotic behavior of the orbits of the Hamiltonian vector field, strongly depends upon the integrability of the Hamiltonian.

Recall that the n-dimensional Hamiltonian h is said to be (Liouville) integrable when there exist n functionally independent first integrals in involution with a certain degree of regularity. When a classical Hamiltonian is integrable, its dynamics is not considered to be chaotic.

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Given an arbitrary classical Hamiltonian there is no algorithmic procedure to ascertain whether it is integrable or not. To our best knowledge, the most general results on this matter are Ziglin's theory [1] and Morales–Ramis' theory [2], which provide criteria to establish that a classical Hamiltonian is not integrable via meromorphic first integrals.

A quantum Hamiltonian H is a self-adjoint linear operator acting on the elements of a separable Hilbert space \mathcal{H} . Proceeding by analogy with the classical case, one can define the dimension (number of degrees of freedom) of a quantum mechanical system [3], obtaining a notion of integrability of a quantum Hamiltonian.

It is said that an n-dimensional Hamiltonian H is integrable when there exist n functionally independent linear operators T_i (i = 1, ..., n) which commute among them and with the Hamiltonian H. In Reference [4] it is proved that this definition is consistent with the classical limit in the sense that if an integrable quantum Hamiltonian possesses a classical counterpart, then it must be integrable as well, although the degree of regularity of its first integrals is not specified. However, there still exist some discrepancies with this definition, as we will discuss in Section 4, since this concept does not have any geometrical content within the framework of Quantum Mechanics.

In Reference [3] it is established a criterion for quantum integrability based on the existence of dynamical symmetries. Unfortunately, the explicit computation of these symmetries is usually complicated. In this paper we provide a sufficient integrability criterion which ensures that every Hamiltonian with pure point spectrum is integrable, allowing a spectral theoretic approach to integrability. Furthermore, this criterion provides a proof (and a precise statement) of a long-standing conjecture of Percival [5].

We also manage to prove that given any closed set of real numbers, there exists an integrable n-dimensional Hamiltonian which realizes it as its spectrum. This result improves a theorem of Crehan [6].

There exists a celebrated conjecture due to Berry [7] which describes the statistical distribution of the point spectrum of a quantum Hamiltonian associated with an integrable classical Hamiltonian [8] and can be stated as follows:

Conjecture 1 (Berry). The point spectrum of a generical quantum system whose Hamiltonian yields a classically integrable system is Poisson distributed.

More specifically [8], the Poisson distribution $P(s) = e^{-s}$ refers to the spacing $s_i = \epsilon_{i+1} - \epsilon_i$ of the normalized energy levels ϵ_i , since the probability

that $s \leq s_i \leq s + ds$ for a random i is P(s) ds. This conjecture has been recently proved for particles subjected to the action of a magnetic field on a flat torus [9].

In this paper we will prove a closely related result ensuring that the statistical distribution of the energy levels of a generic quantum Hamiltonian with pure point spectrum is also Poissonian. We also prove that for each unitary class of Hamiltonians with pure point spectrum there exists a representative to which Conjecture 1 applies. This fact can be considered a different but analogous, physically meaningful statement which describes a purely quantum mechanical version of Conjecture 1 without appealing to the semiclassical approximation and which provides additional support for Berry's conjecture.

This paper is organized as follows. In Section 2 the integrability of Hamiltonians with pure point spectrum is studied, obtaining additional results on the existence of integrable Hamiltonians realizing certain prescribed spectrum in arbitrary dimension. In Section 3 we use this results to gain some insight into Berry's conjecture. Finally, other interesting consequences of this new integrability criterion are given in Section 4, and a critical discussion of the concept of quantum integrability is presented based on the discrepancies of its standard definition and general wisdom, and on its lack of geometric content.

2 Integrability of Hamiltonians with pure point spectrum

In this section we will establish the integrability of any n-dimensional Hamiltonian H whose continuous spectrum is empty. Our proof will rest upon the explicit construction of an integrable self-adjoint operator A which is completely isospectral to our Hamiltonian H in the following sense.

Definition 1. Two self-adjoint operators A and H are completely isospectral when $\sigma_{\text{cont}}(A) = \sigma_{\text{cont}}(H)$, $\sigma_{\text{pp}}(A) = \sigma_{\text{pp}}(H)$ and the eigenvalues of A and H present the same multiplicities.

The definition of point spectrum which we will use in this article is that of [10]: λ is in $\sigma_{pp}(A)$ if and only if it is an eigenvalue of the self-adjoint operator A. We also use the direct sum decomposition $\mathcal{H} = \mathcal{H}_{pp} \oplus \mathcal{H}_{cont}$ [10],

and define $\sigma_{\text{cont}}(A) = \sigma(A|_{\mathcal{H}_{\text{cont}}})$. This provides the decomposition

$$\sigma(A) = \overline{\sigma_{\rm pp}(A)} \cup \sigma_{\rm cont}(A)$$
,

where these two sets are not necessarily disjoint. The self-adjoint operator A will be said to have pure point spectrum when $\sigma_{\text{cont}}(A) = \emptyset$. In this paper, the overline will represent the closure of a set and \mathbb{N}_0 will stand for the set $\{0, 1, 2, \ldots\}$.

Given a sequence $C = (E_i)_{i \in \mathbb{N}_0}$ of real numbers, with possibly repeated elements, we shall consider the associated set

$$C = \bigcup_{i \in \mathbb{N}_0} \{ E_i \}$$

of the values taken in this sequence.

Definition 2. A self-adjoint operator A is said to realize the sequence C as its spectrum if $\sigma_{\text{cont}}(A) = \emptyset$, $\sigma_{\text{pp}}(A) = C$ and the multiplicity of each eigenvalue E of A equals the times it appears in C, i.e., $\text{card}\{i \in \mathbb{N}_0 \mid E_i = E\}$.

This definition clearly implies that $\sigma(A) = \overline{C}$. Now we will concentrate on the construction of an integrable Hamiltonian realizing a prescribed sequence $\mathcal{C} \subset \mathbb{R}$ as its spectrum. We will follow Crehan's approach to this problem [6].

We will need the following elementary lemma, whose proof is straightforward and will be omitted.

Lemma 1. Let $C = (E_i)_{i \in \mathbb{N}_0}$ be a sequence. Then there exists a C^{∞} function $f : \mathbb{R}^n \to \mathbb{R}$ and a bijection $\phi : \mathbb{N}_0^n \to \mathbb{N}_0$ such that $f(I) = E_{\phi(I)}$ for all $I \in \mathbb{N}_0^n$.

In fact, combining the theorems of Mittag-Leffler and Weierstrass one can prove ([11], Theorem 15.15) that f can actually be chosen to be entire whenever \mathcal{C} does not possess any accumulation points.

Proposition 1. Let C be a sequence of real numbers. Then there exists an integrable n-dimensional Hamiltonian A, whose n commuting first integrals can be chosen to be self-adjoint, which realizes the sequence C as spectrum.

Proof. Let f be a function as in Lemma 1. Let $N_i = \frac{1}{2}(X_i^2 + P_i^2 - 1)$ (i = 1, ..., n) be the number operator associated with the *i*-th coordinate.

It is clear that these number operators commute among them: $[N_i, N_j] = 0$. Let us define A by

$$A = f(N_1, \dots, N_n),$$

for instance, via continuous functional calculus. Since the number operators N_i $(i=1,\ldots,n)$ are self-adjoint and commute among them, we conclude that A is also self-adjoint and that it commutes with the number operators. These number operators are obviously functionally independent and therefore they constitute a complete family of commuting self-adjoint first integrals of the Hamiltonian A.

The fact that these number operators act on different coordinates also enables us to compute the spectrum of A readily: its point spectrum $\sigma_{pp}(A)$ is, by construction, C; its continuous spectrum is empty; and the fact that $f(I) = E_{\phi(I)}$ for all $I \in \mathbb{N}_0^n$, ϕ being a bijection, forces the multiplicity of each eigenvalue to be given by the formula in Definition 2.

Remark 1. It is interesting to observe that every C^{∞} extension f of the mapping $I \in \mathbb{N}_0^n \mapsto E_{\phi(I)} \in C$ gives raise to the same quantum Hamiltonian A. However, different choices of this extension f lead to different classical Hamiltonians via the substitution $a_f(x,p) = f(\frac{1}{2}(x_1^2 + p_1^2 - 1), \dots, \frac{1}{2}(x_n^2 + p_n^2 - 1))$. Therefore we have an uncountable family of different classically integrable n-dimensional Hamiltonians yielding the same integrable quantum Hamiltonian. Note that all the orbits of these classical Hamiltonians are bounded and generally dense on n-dimensional tori.

Remark 2. A classical Hamiltonian h whose dependence on its variables is of the form $h = h(x_1^2 + p_1^2, \dots, x_n^2 + p_n^2)$ is said to appear in Birkhoff normal form. It is well known that every analytic integrable classical Hamiltonian satisfying certain mild technical conditions may be cast into this form [12].

Proposition 1 can be used to prove the existence of an integrable Hamiltonian whose spectrum is any closed set $\Sigma \subset \mathbb{R}$. Let us recall the following lemma.

Lemma 2. Let $\Sigma \subset \mathbb{R}$ be a closed set. Then there exists a countable set $C \subset \Sigma$ which is dense in Σ .

Proof. Since complete separability is hereditary and \mathbb{R} , endowed with its usual metric topology, is completely separable, so is Σ . Complete separability implies separability, so the lemma is proved.

The existence of the desired Hamiltonian now stems from previous results.

Proposition 2. Let $\Sigma \subset \mathbb{R}$ be a closed set. Then there exists an integrable n-dimensional Hamiltonian A such that $\sigma(A) = \Sigma$ and $\sigma_{\text{cont}}(A) = \emptyset$. Besides, its n commuting, functionally independent first integrals can be chosen to be self-adjoint.

Proof. By Lemma 3, there exists a countable set $C = \{c_i\} \subset \Sigma$ that is dense in Σ . Application of Proposition 1 to the sequence $\mathcal{C} = (c_i)$ yields the desired result.

These results can be used to establish the integrability of any Hamiltonian H with pure point spectrum. Let us start proving an auxiliary lemma.

Lemma 3. Let A and H be two self-adjoint, completely isospectral operators with pure point spectrum. Then they are unitarily equivalent.

Proof. Let $C = (E_i)_{i \in \mathbb{N}_0}$ be a sequence such that $C = \sigma_{pp}(A) = \sigma_{pp}(H)$, each eigenvalue appearing as many times as its multiplicity. Since H is self-adjoint and its continuous spectrum is empty, one can choose an orthonormal basis of eigenfunctions of H, $\mathcal{B}_H = \{e_i \mid i \in \mathbb{N}_0\}$, such that $He_i = E_ie_i$. The same reasoning provides an orthonormal basis of eigenfunctions of A, $\mathcal{B}_A = \{\hat{e}_i \mid i \in \mathbb{N}_0\}$, such that $A\hat{e}_i = E_i\hat{e}_i$. Set $Ue_i = \hat{e}_i \ (i \in \mathbb{N}_0)$ and extend U by linearity. Then U is a unitary transformation and satisfies UH = AU. \square

The following theorem, new in the literature, improves the results in Crehan [6] and Weigert [13].

Theorem 1. Let H be an n-dimensional Hamiltonian with pure point spectrum. Then it is integrable and its n commuting first integrals can be chosen to be self-adjoint.

Proof. By Proposition 1, we can construct an integrable n-dimensional Hamiltonian A that is completely isospectral to H and with n functionally independent, commuting, self-adjoint first integrals N_1, \ldots, N_n . By Lemma 3, there exists a unitary transformation U such that $H = U^{\dagger}AU$. Then the operators $T_i = U^{\dagger}N_iU$ $(i = 1, \ldots, n)$ constitute a complete set of functionally independent, commuting, self-adjoint first integrals.

Remark 3. The physical interest of this theorem is laid bare noting that these operators are dense in the set of self-adjoint operators: for every n-dimensional Hamiltonian H there exists a family of Hamiltonian operators $\{H_i\}_{i\in\mathbb{N}}$ such that H_i has pure point spectrum (and is, therefore, integrable) and $||H - H_i|| \to 0$. The proof is a straightforward application of the properties of the spectral family of H.

Remark 4. Despite the results of Zhang et al. [3, 4], it is not obvious the connection between quantum and classical integrability. We have not proved any regularity conditions of the classical counterparts $t_i(x, p)$ of the quantum first integrals T_i (i = 1, ..., n), so we cannot claim that a classical dynamical system whose quantum mechanical counterpart has pure point spectrum must be integrable in any usual sense, i.e., via analytic, meromorphic or smooth first integrals.

Let us consider the following example. Let (M,g) be a compact Riemannian manifold. Let $H=-\Delta$ be the Hamiltonian of a free particle in M, where Δ represents the Laplace-Beltrami operator. An appropriate choice of the domain $\mathrm{D}(H)\subset L^2(M)$ leads to a self-adjoint operator whose spectrum is known to be discrete [14] and therefore quantum integrable. The theorem of Matveev and Topalov [15] on quantum integrability of Laplacians on closed manifolds with non-proportional geodesically equivalent metrics is thus extended to any closed manifold using Theorem 1.

However, the classical dynamical system associated to this Hamiltonian $H=-\Delta$, whose equation of motion is just the geodesic equation, is generally non-integrable in any usual sense. In fact, Anosov [16, 17] proved that this equation cannot be integrable via continuous first integrals in any compact Riemannian manifold of strictly negative sectional curvature.

It is also worth mentioning another famous example of this phenomenon. The potential $V(x,y)=x^2y^2$ in \mathbb{R}^2 is known to have discrete spectrum [18], so $H=-\partial_x^2-\partial_y^2+V(x,y)$ is integrable. However, its associated classical Hamiltonian $h=p_x^2+p_y^2+V(x,y)$ is non-integrable via analytic functions as a consequence of Yoshida's criterion [19], and in fact numerical explorations show a complex orbit structure.

One ought to note that these examples should not be regarded as exceptional, since in fact this will be the general case. This is due to the fact that the unitary transformations that appear in the quantum case do not induce symplectomorphisms of the classical counterparts. This situation can be clearly observed in the examples above, where the quantum Hamiltonian

has been shown to be unitarily equivalent to an integrable Hamiltonian in Birkhoff's normal form but their classical analogues are non-integrable and cannot be transformed into this form using a symplectomorphism.

An easy, physically significant corollary can be immediately derived from this sufficient integrability condition.

Corollary 1. Let H be an n-dimensional Hamiltonian. When its spectrum is countable, it is integrable and its n commuting first integrals can be chosen to be self-adjoint.

Proof. According to Theorem 1 and the definition of continuous spectrum, it is enough to prove that $\mathcal{H}_{cont} = \{0\}$. Recall that $\psi \in \mathcal{H}_{cont}$ if and only if its spectral measure μ_{ψ} is continuous with respect to the Lebesgue measure [10]. The formula

$$(\psi, f(H)\psi) = \int f(\lambda) d\mu_{\psi}(\lambda),$$

applied to $f(\lambda) = 1$, and the fact that supp $\mu_{\psi} \subset \sigma(H)$ then combine to show that $\|\psi\| = 0$ for all $\psi \in \mathcal{H}_{cont}$.

3 Statistical distribution of Hamiltonians with pure point spectrum

Let S_n be the class of unitarily equivalent n-dimensional Hamiltonians with pure point spectrum. Note that each element belonging to this class is uniquely specified by its sequence of eigenvalues C up to unitary equivalence. Theorem 1 shows that all the Hamiltonians in this class are integrable. In Remark 1 it was stated that for each class in S_n there exists a representative which has a (non-unique) smooth, integrable classical analogue.

Let $C = (\epsilon_i)_{i \in \mathbb{N}_0}$ be the sequence of normalized energies of a certain integrable Hamiltonian. The way in which this normalization must be carried out is carefully explained in [8]. It is well known that Berry and Tabor [7] conjectured that the statistical distribution of the differences of normalized energies is generically Poissonian. In Theorem 2 an analogous property for standard, Hilbert-space Quantum Mechanics is proved for S_n . Although clearly resembling Berry's conjecture, this theorem is of a purely quantum mechanical nature and does not refer to any semiclassical limit of the quantum Hamiltonian. Nevertheless, this theorem is mathematically rigorous and physically interesting in its own right.

It is enlightening to observe that however this theorem does provide additional support for Berry's conjecture since Remark 1 ensures that for each unitary class in S_n there exists a smooth, classically integrable Hamiltonian h to which Berry's conjecture applies.

Since it is readily shown that the set of normalized energy differences is Poisson distributed when the set of normalized energies follows the uniform distribution, as proved in [8], our results on uniform distribution of energies can be stated as follows.

Theorem 2. For almost all Hamiltonians belonging to the class S_n , its point spectrum is uniformly distributed.

Proof. The previous lemma implies that an element of S_n is specified by a sequence of real numbers C up to a change of orthonormal basis, i.e., the classes of operators in S_n are in a one to one correspondence with the sequences of real numbers. It is known that the set of all uniform distributed sequences in a compact space has full measure, i.e., its complement has Lebesgue measure zero [20]. Although we have sequences of reals, we can compactify \mathbb{R} . Since the sequences in \mathbb{R} in which at least one element takes the value $+\infty$ or $-\infty$ have measure zero, we reach the result that almost all (classes of) Hamiltonians in S_n verify the statement.

4 Final remarks and discussion

In this paper we have obtained a new integrability criterion based on the spectral properties of a quantum Hamiltonian, and proved a result on the spectral distribution of integrable quantum Hamiltonians which resembles a purely quantum version of Berry's conjecture. It is important to remark that these results are obtained in a purely quantum mechanical setting, and do not rest upon any semiclassical treatment. It would be interesting to develop a complete characterization of integrable self-adjoint operators in terms of their spectrum, that is, an equivalence between integrability and certain properties of the spectrum, and explore the relationship between Theorem 2 and Berry's conjecture.

A straightforward consequence of Theorem 1 is that non-integrable quantum Hamiltonians must possess uncountable spectra. Following the terminology of Percival [5], our theorem implies that regular spectra (that is, spectra given by smooth functions of the quantum numbers) can only be realized by

integrable quantum Hamiltonians since regular spectra are always countable. That a regular spectrum corresponds to integrability is a long-standing conjecture of Percival for which Theorem 1 provides a proof in a purely quantum setting.

Another open question in the literature [21] is the study of Hamiltonians whose point spectrum is given by the real solutions c_i $(i \in \mathbb{N})$ of

$$\zeta(\frac{1}{2} + \mathrm{i}c_i) = 0,$$

where ζ is the Riemann Zeta function. Its interest is due to the fact that the statistics associated to the energy levels spacing of $(c_i)_{i\in\mathbb{N}}$ is GUE and this statistics is generically associated to quantum chaos. Theorem 1 implies that any n-dimensional quantum Hamiltonian with spectrum given by $(c_i)_{i\in\mathbb{N}}$ must be integrable, improving a result of Crehan [6] which ensures the existence of an integrable quantum Hamiltonian realizing $(c_i)_{i\in\mathbb{N}}$ as its spectrum. It should be noticed that, as already mentioned, our theorems do not prove classical integrability, since they provide purely quantum mechanical results. Actually some of these Hamiltonians are known to have non-integrable classical counterparts, and therefore quantum chaos may appear within the context of semiclassical Quantum Mechanics.

As another nontrivial application of our integrability criterion, we will establish the integrability of the movement of a quantum particle in \mathbb{R}^n in a lower bounded potential V such that $V(x) \to +\infty$ as $x \to \infty$. Let us consider a lower bounded potential $V \in L^r_{loc}(\mathbb{R}^n)$ $(r > \min\{2, \frac{n}{2}\})$ such that

$$\lim_{R \to 0} \sup_{x \in \mathbb{R}^n} \int_{|x-y| < R} |x-y|^{4-n-\epsilon} V(y)^2 d^n y = 0$$

for some $\epsilon > 0$ and the Hamiltonian $H = -\Delta + V(x)$, defined on

$$D(H) = \left\{ \psi \in L^2(\mathbb{R}^n) \mid \Delta \psi \in L^2(\mathbb{R}^n) \right\},\,$$

where the derivatives are to be understood in a distributional sense [22].

Theorem 3. Let the n-dimensional Hamiltonian $H = -\Delta + V(x)$ be defined as above, and suppose that $V(x) \to +\infty$ as $x \to \infty$. Then H is integrable via self-adjoint first integrals.

Proof. In Reference [22] it is proved that H is self-adjoint and its spectrum is discrete. Hence Corollary 1 implies that H is integrable.

Remark 5. As stated in Remark 4, the quantum mechanical integrability of the Hamiltonian $H = P^2 + V(X)$ in \mathbb{R}^n under the aforementioned hypothesis does not imply the integrability of its classical analogue via smooth first integrals. It cannot be claimed that Theorem 3 provides a proof for this statement in the context of Classical Mechanics, and actually some examples are known [23] in which a potential as described above gives raise to a classical Hamiltonian which is not integrable via meromorphic functions.

We will end up with a short digression on the validity of our results. First we should note that some authors believe [24, 25] that Quantum Mechanics is always completely integrable, in some sense. A simple argument goes as follows: let H be a Hamiltonian and let $\{P_{\Omega}\}$ be its projection valued measure [10]. Then, for a generic Hamiltonian, there exists a partition \mathcal{B} of $\sigma(H)$ into measurable sets whose pairwise intersections have measure zero such that $\{P_{\Omega} \mid \Omega \in \mathcal{B}\}$ is an infinite family of commuting, self-adjoint, functionally independent first integrals of H. Hence Quantum Mechanics is generically superintegrable according to the definition which we have used in this article, which is also the most popular one in the literature.

Although we do not intend to present here a detailed study of quantum integrability, we will point out that the results obtained in this paper are not vacuous, since, actually, we have been implicitly using the following stronger definition of integrability, which in fact closely resembles the definition proposed in [26] in the context of (finite-dimensional) spin dynamics.

Definition 3. An *n*-dimensional Hamiltonian H is integrable when it is unitarily equivalent to a self-adjoint operator A, defined on a dense subset of $L^2(\mathbb{R}^n)$, which possesses n commuting, self-adjoint, functionally independent first integrals N_1, \ldots, N_n such that both A and these N_i are smooth functions of the operators $(X\psi)(x) = x\psi(x)$ and $(P\psi)(x) = -i\nabla\psi(x)$.

In more physical terms, we consider that a quantum n-dimensional Hamiltonian is integrable when it can be obtained from a canonically quantized, classically integrable Hamiltonian system in \mathbb{R}^n via a change of orthonormal basis. This definition ensures the nontriviality of our theorems.

The results of this paper arise the question of to what extent the concept of quantum integrability can be given a non-vacuous meaning. In Classical Mechanics this notion, when suitably defined, merely reflects the geometric simplicity of the orbit structure of the Hamiltonian system. However, the standard definition of quantum integrability, which follows naively from this

classical concept, or even the slightly stronger one provided in Definition 3, does not possess any geometric content, and therefore cannot be regarded as the quantum analogue of classical integrability. In light of these remarks, the formal obstructions to the standard definition of quantum integrability raised by the celebrated theorem of Von Neumann on commuting sets of self-adjoint operators [27] are hardly surprising. In this view one can also understand the amazing fact that, as stated in Remark 3, integrable n-dimensional Hamiltonians are dense in the set of self-adjoint operators, while it is well known [28] that classically integrable Hamiltonians are nowhere dense.

There remains as an open question to define a meaningful, geometrically significant notion of quantum integrability, which probably would be related to the orbit structure in the projective Hilbert space of the quantum system and is expected to reproduce those aspects of quantum integrability which are nowadays common knowledge even though they are not compatible with the standard definition of quantum integrability, establishing a clear physical distinction between the behaviors of an integrable and a non-integrable system. It would come to no surprise that a geometrical definition following this philosophy were finally independent of the number of degrees of freedom of the system, since in fact the Hilbert spaces $\mathcal{H}_{N,n}$ describing the dynamics of N quantum particles of arbitrary spin moving in \mathbb{R}^n are isomorphic for every choice of N, n and the spins. An important step towards the understanding of the concept of quantum integrability in geometrical terms is due to Cirelli and Pizzocchero [24], but many important questions in this field are still unanswered.

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